NATIONAL ENERGY TECHNOLOGY LABORATORY

MPPIC model implementation in MFIX: frictional solid-stress model

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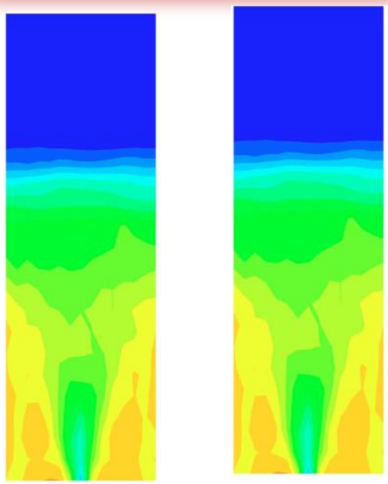
U.S. DEPARTMENT OF ENERGY

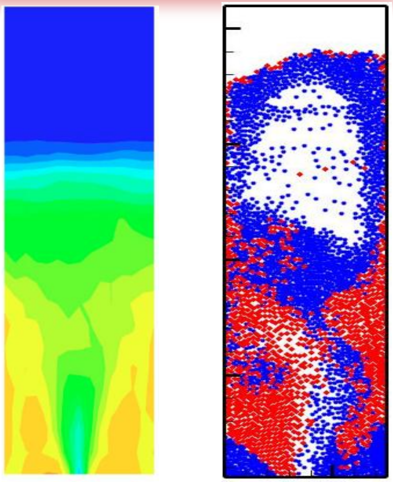
Current simulation types in MFIX

EE simulations



Fluid *Solid*

EL simulations



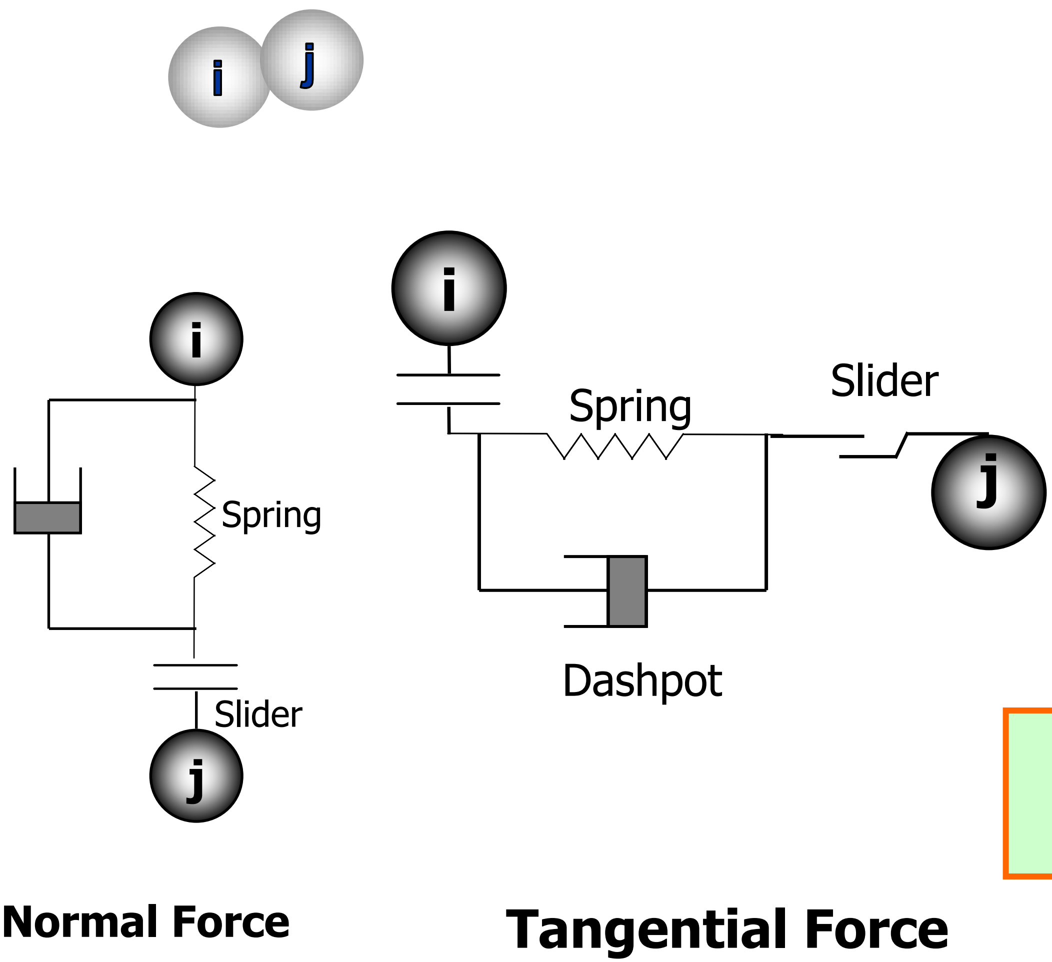
Fluid *Solid*

- ❑ **Two-Fluid Method (Volume/Ensemble averaging)**
- ❑ **Quadrature methods (discretized distribution function)**

- ❑ **Discrete-element method (MFIX-DEM)**
- ❑ **Multiphase-Particle-In-Cell method (MPPIC), DPM, dense-phase-DPM, etc.**

Discrete Element Method (DEM)

Collision between real particles



Advantages

- Collisions directly resolved
- Tool for model validation

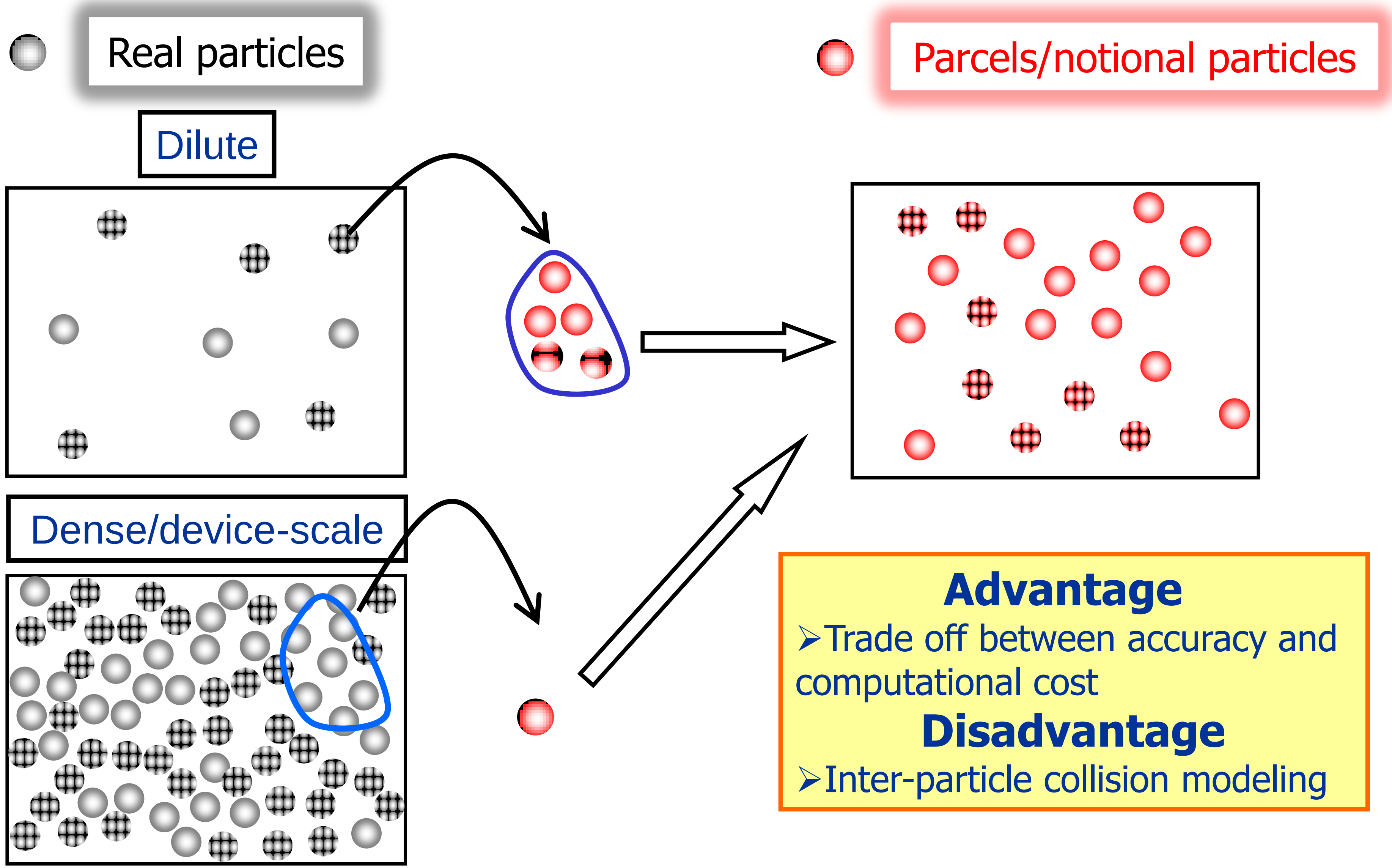
Disadvantages

- Impractical for large-scale problems
- Not ideal for distributed memory parallelization

Remedy

Use parcels/notional particles

MPPIC model



Advantage

- ➢Trade off between accuracy and computational cost

Disadvantage

- ➢Inter-particle collision modeling

MPPIC: current state-of-the-art

- ✓ **MPPIC model is a useful tool for quick turnaround simulations of engineering applications (*2006 roadmap*)**
- ✓ **Several commercial implementations (Barracuda by CPFD, Dense-phase-DPM by ANSYS)**
- ✓ **Hard to ascertain and further develop sub-models (such as collision, friction, etc.)**
- ✓ **Lack of an open-source implementation that can be used for model development/enhancement, and independent verification and validation (V&V)**
- ➢ ***Objective of this study:* Implement MPPIC like model in open-source MFIX code to probe its accuracy and speed**

MPPIC model details

Carrier Phase: averaged Navier-Stokes equation

$$\frac{\partial(\varepsilon_{\mathrm{g}}\rho_{\mathrm{g}})}{\partial t} + \nabla \cdot (\varepsilon_{\mathrm{g}}\rho_{\mathrm{g}}\mathbf{v}_{\mathrm{g}}) = 0$$

$$\frac{D}{Dt}(\varepsilon_{\mathrm{g}}\rho_{\mathrm{g}}\mathbf{v}_{\mathrm{g}}) = \nabla \cdot \overline{\overline{S}}_{\mathrm{g}} + \varepsilon_{\mathrm{g}}\rho_{\mathrm{g}}\mathbf{g} - \mathbf{F}_{\mathrm{drag}}$$

$\mathbf{A}_{\mathrm{coll}}$ is the collision operator used to model collisions in the ***kinetic*** and ***frictional*** regimes.

Robust implementation of ***frictional regime*** $\mathbf{A}_{\mathrm{coll}}$ is critical to stability of MPPIC model

Dispersed Phase

$$\frac{d\mathbf{x}_{\mathrm{p}}}{dt} = \mathbf{u}_{\mathrm{p}}$$

$$m\frac{d\mathbf{u}_{\mathrm{p}}}{dt} = m\mathbf{g} + \mathbf{f}_{\mathrm{p,drag}} + m\mathbf{A}_{\mathrm{coll}}$$

Particle trajectory evolution

$$\boxed{m\frac{d\mathbf{u}_{\mathrm{p}}}{dt} = m\mathbf{g} + \mathbf{f}_{\mathrm{p,drag}} + m\mathbf{A}_{\mathrm{coll}}}$$

$$\mathbf{u}'^{n+1}_{\mathrm{p}} = \mathbf{u}^{n}_{\mathrm{p}} + \left(\mathbf{g} + \frac{\mathbf{f}_{\mathrm{p,drag}}}{m}\right)\Delta t$$

$$\mathbf{x}'^{n+1}_{\mathrm{p}} = \mathbf{x}^{n}_{\mathrm{p}} + \Delta t\,\mathbf{u}'^{n+1}_{\mathrm{p}}$$

$$\left(\mathbf{x}'^{n+1}_{\mathrm{p}}, \mathbf{u}'^{n+1}_{\mathrm{p}}\right) \xrightarrow[\text{Specular}]{\text{Wall B.C.}} \left(\mathbf{x}^{n+1}_{\mathrm{p}}, \mathbf{u}^{*n+1}_{\mathrm{p}}\right)$$

$$\mathbf{u}^{*n+1}_{\mathrm{p}} \xrightarrow{A_{\mathrm{coll}}} \mathbf{u}^{n+1}_{\mathrm{p}}$$

How is A_{coll} applied ?

A_{coll} implementation (frictional regime)

$$\boxed{m\frac{d\mathbf{u}_{\text{p}}}{dt} = m\mathbf{g} + \mathbf{f}_{\text{p,drag}} + m\mathbf{A}_{\text{coll}}}$$

$$\mathbf{u}'^{n+1}_{\text{p}} = \mathbf{u}^{n}_{\text{p}} + \left(\mathbf{g} + \frac{\mathbf{f}_{\text{p,drag}}}{m}\right)\Delta t$$

$$\mathbf{x}'^{n+1}_{\text{p}} = \mathbf{x}^{n}_{\text{p}} + \Delta t \mathbf{u}'^{n+1}_{\text{p}}$$

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$$\mathbf{u}^{*n+1}_{\text{p}} \xrightarrow{A_{\text{coll}}} \mathbf{u}^{n+1}_{\text{p}}$$

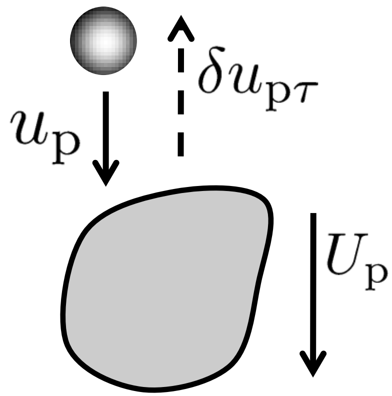
$$\chi = \varepsilon_{\text{s}} \quad \varepsilon_{\text{s}} \geq \varepsilon_{\text{s}_{\text{cp}}}$$
$$= 0 \quad \text{otherwise}$$

$$\delta\mathbf{u}_{\text{p}\tau} = -\nabla\chi$$

χ is like a coloring function used to indicate the close-packed regions. $\delta\mathbf{u}_{\text{p}\tau}$ is non-zero inside *and* at the interfaces of close-packed regions. It only indicates the direction of the correction due to close-packing.

A_{coll} implementation

Case 1



U_p: average solids velocity

if $|u_p| > |U_p|$

REBOUND

$$u_p^{n+1} = -e\, u_p$$

else

DO NOTHING

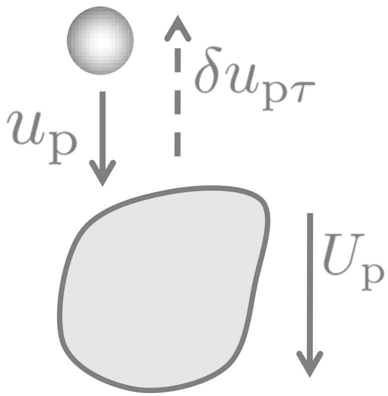
$$\mathbf{u}^{*n+1}_p \xrightarrow{A_{coll}} \mathbf{u}^{n+1}_p$$

$$\chi = \varepsilon_s \quad \varepsilon_s \geq \varepsilon_{s_{cp}}$$
$$= 0 \quad \text{otherwise}$$

$$\delta \mathbf{u}_{p\tau} = -\boldsymbol{\nabla}\chi$$

A_{coll} implementation

Case 1



if $|u_{\mathrm{p}}| > |U_{\mathrm{p}}|$

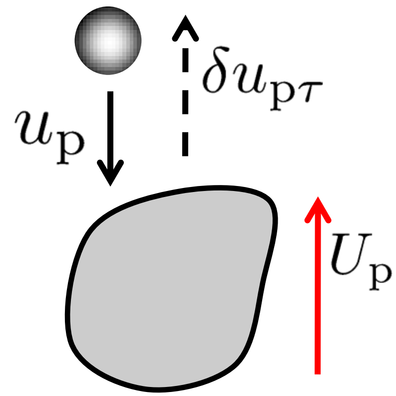
REBOUND

$$u_{\mathrm{p}}^{n+1} = -e\, u_{\mathrm{p}}$$

else

DO NOTHING

Case 2



REBOUND

$$u_{\mathrm{p}}^{n+1} = -e\, u_{\mathrm{p}}$$

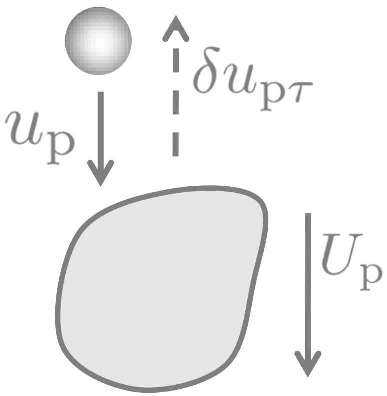
$$\mathbf{u}^{*n+1}_{\mathrm{p}} \xrightarrow{A_{\text{coll}}} \mathbf{u}_{\mathrm{p}}^{n+1}$$

$$\chi = \begin{cases} \varepsilon_{\mathrm{s}} & \varepsilon_{\mathrm{s}} \geq \varepsilon_{\mathrm{scp}} \\ 0 & \text{otherwise} \end{cases}$$

$$\delta \mathbf{u}_{\mathrm{p}\tau} = -\boldsymbol{\nabla} \chi$$

A_{coll} implementation

Case 1



if $|u_p| > |U_p|$

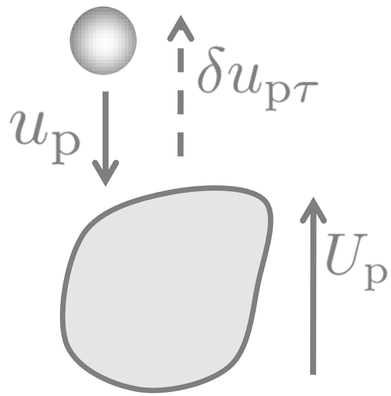
REBOUND

$$u_p^{n+1} = -e\, u_p$$

else

DO NOTHING

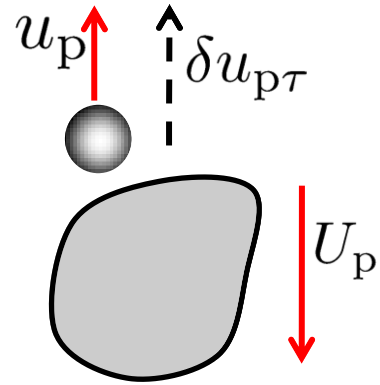
Case 2



REBOUND

$$u_p^{n+1} = -e\, u_p$$

Case 3



DO NOTHING

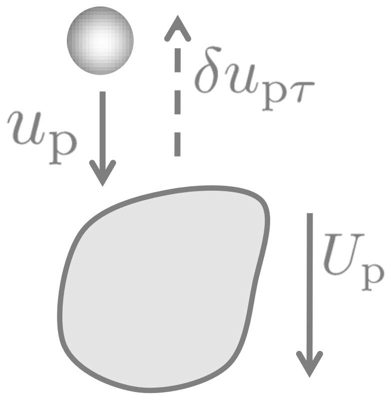
$$\mathbf{u}_p^{*n+1} \xrightarrow{A_{coll}} \mathbf{u}_p^{n+1}$$

$$\chi = \varepsilon_s \quad \varepsilon_s \geq \varepsilon_{s\,cp}$$
$$= 0 \quad \text{otherwise}$$

$$\delta \mathbf{u}_{p\tau} = -\boldsymbol{\nabla}\chi$$

A_{coll} implementation

Case 1



if $|u_p| > |U_p|$

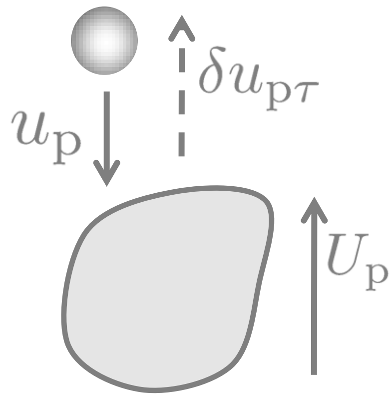
REBOUND

$$u_p^{n+1} = -e\, u_p$$

else

DO NOTHING

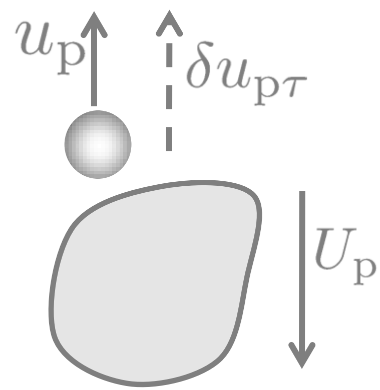
Case 2



REBOUND

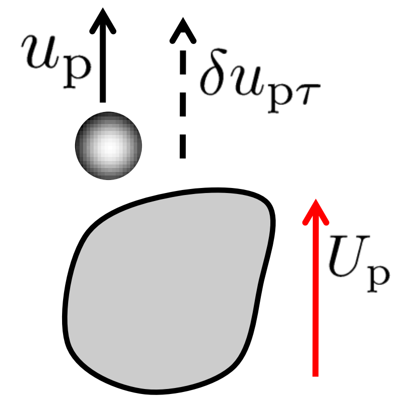
$$u_p^{n+1} = -e\, u_p$$

Case 3



DO NOTHING

Case 4



DO NOTHING

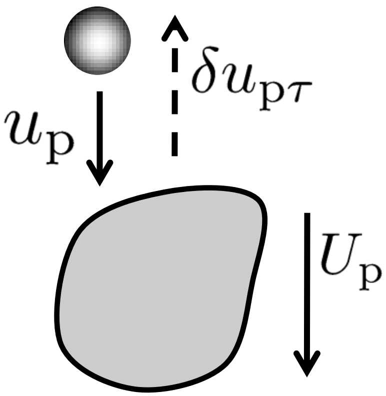
$$\mathbf{u}^{*\,n+1}_{\mathrm{p}} \xrightarrow{A_{\text{coll}}} \mathbf{u}^{n+1}_{\mathrm{p}}$$

$$\chi = \varepsilon_{\mathrm{s}} \qquad \varepsilon_{\mathrm{s}} \geq \varepsilon_{\mathrm{s}_{\mathrm{cp}}}$$
$$= 0 \qquad \text{otherwise}$$

$$\delta \mathbf{u}_{\mathrm{p}\tau} = -\nabla \chi$$

A_{coll} implementation

Case 1



if $|u_p| > |U_p|$

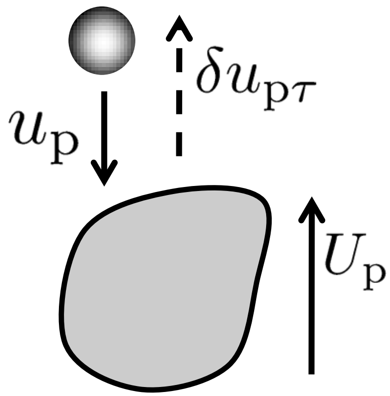
REBOUND

$$u_p^{n+1} = -e\,u_p$$

else

DO NOTHING

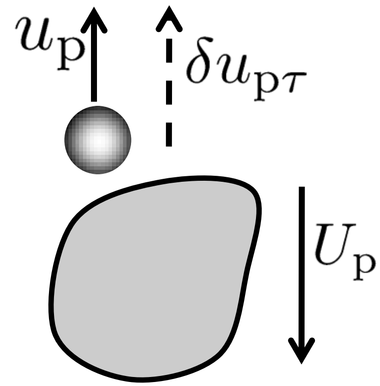
Case 2



REBOUND

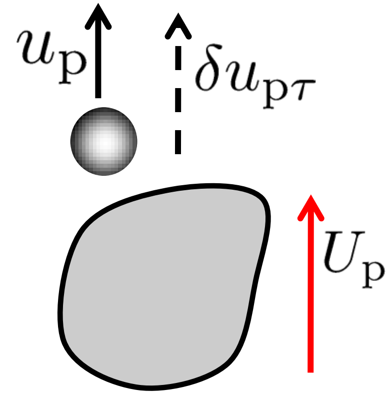
$$u_p^{n+1} = -e\,u_p$$

Case 3



DO NOTHING

Case 4



DO NOTHING

$$\mathbf{u}_p^{*n+1} \xrightarrow{A_{\text{coll}}} \mathbf{u}_p^{n+1}$$

$$\chi = \begin{cases} \varepsilon_s & \varepsilon_s \geq \varepsilon_{s_{cp}} \\ 0 & \text{otherwise} \end{cases}$$

$$\delta \mathbf{u}_{p\tau} = -\nabla \chi$$

Comparison with existing literature

$$\boxed{m\frac{d\mathbf{u}_\mathrm{p}}{dt} = m\mathbf{g} + \mathbf{f}_\mathrm{p,drag} + m\mathbf{A}_\mathrm{coll}}$$

$$\mathbf{u}_\mathrm{p}^{n+1} = \widetilde{\mathbf{u}}_\mathrm{p} + \mathbf{u}_{\mathrm{p}\tau}$$

$$\widetilde{\mathbf{u}}_\mathrm{p} = \mathbf{u}_\mathrm{p}^{n} + \left(\mathbf{g} + \frac{\mathbf{f}_\mathrm{p,drag}}{m}\right)\Delta t$$

No inter-particle collision term so far

Snider, D. M., An incompressible 3-D MP-PIC model for dense particle flows, JCP (2001)

Comparison with existing literature

$$m\frac{d\mathbf{u}_{\mathrm{p}}}{dt} = m\mathbf{g} + \mathbf{f}_{\mathrm{p,drag}} + m\mathbf{A}_{\mathrm{coll}}$$

$$\mathbf{u}_{\mathrm{p}}^{n+1} = \tilde{\mathbf{u}}_{\mathrm{p}} + \mathbf{u}_{\mathrm{p}\tau}$$

$$\tau = \frac{P_{\mathrm{s}}\varepsilon_{\mathrm{s}}^{\beta}}{\max\left[\varepsilon_{\mathrm{scp}} - \varepsilon_{\mathrm{s}}, \epsilon\left(1 - \varepsilon_{\mathrm{s}}\right)\right]}$$

Isotropic inter-particle stress (Harris and Crighton)

$$\delta\mathbf{u}_{\mathrm{p}\tau} = -\frac{\Delta t \boldsymbol{\nabla}\tau}{\rho_{\mathrm{s}}\varepsilon_{\mathrm{s}}}$$

Decides the direction of solid-stress correction velocity

$$(\boldsymbol{\nabla}\tau).\mathbf{e}_k \leq 0$$

$$u'_{p\tau k} = \min\left(\mathbf{e}_k \cdot \delta\mathbf{u}_{\mathrm{p}\tau}, (1+\gamma)(\mathbf{U}_p - \tilde{\mathbf{u}}_{\mathrm{p}}) \cdot \mathbf{e}_k\right)$$

$$u_{p\tau k} = \max\left(u'_{p\tau k}, 0\right)$$

Matters mostly near close-packing, otherwise statistical noise!

Comparison with existing literature

$$m\frac{d\mathbf{u}_{\mathsf{p}}}{dt} = m\mathbf{g} + \mathbf{f}_{\mathsf{p,drag}} + m\mathbf{A}_{\mathsf{coll}}$$

$$\mathbf{u}_{\mathsf{p}}^{n+1} = \tilde{\mathbf{u}}_{\mathsf{p}} + \mathbf{u}_{\mathsf{p}\tau}$$

$$\tau = \frac{P_{\mathsf{s}}\varepsilon_{\mathsf{s}}^{\beta}}{\max\left[\varepsilon_{\mathsf{scp}} - \varepsilon_{\mathsf{s}}, \epsilon\left(1 - \varepsilon_{\mathsf{s}}\right)\right]}$$

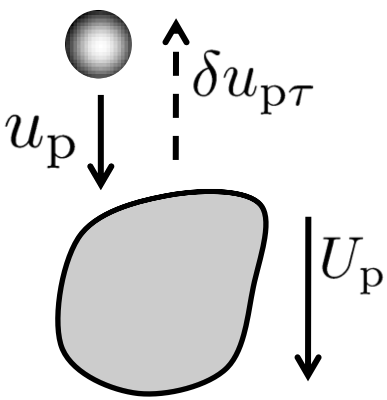
$$\delta\mathbf{u}_{\mathsf{p}\tau} = -\frac{\Delta t \boldsymbol{\nabla}\tau}{\rho_{\mathsf{s}}\varepsilon_{\mathsf{s}}}$$

$$\boxed{\begin{aligned} &(\boldsymbol{\nabla}\tau).\mathbf{e}_k \leq 0 \\ &u'_{p\tau_k} = \min\left(\mathbf{e}_k \cdot \delta\mathbf{u}_{\mathsf{p}\tau}, (1+\gamma)(\mathbf{U}_p - \tilde{\mathbf{u}}_{\mathsf{p}}) \cdot \mathbf{e}_k\right) \\ &u_{p\tau_k} = \max\left(u'_{p\tau_k}, 0\right) \end{aligned}}$$

WHAT DO THESE LIMITERS IMPLY ?

Explanation of limiters

Case 1



if $|u_p| > |U_p|$

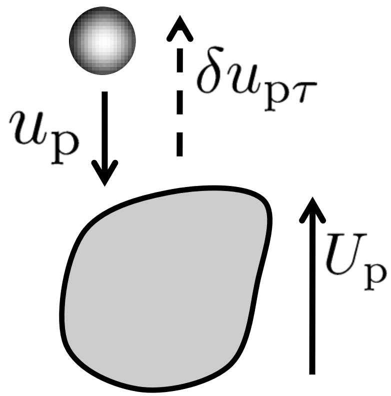
REBOUND

$u_{p\tau} = (1+\gamma)(U_p - u_p)$

else

DO NOTHING

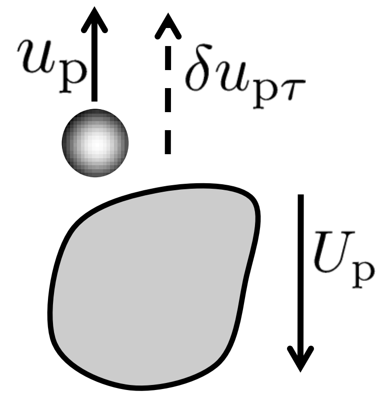
Case 2



REBOUND

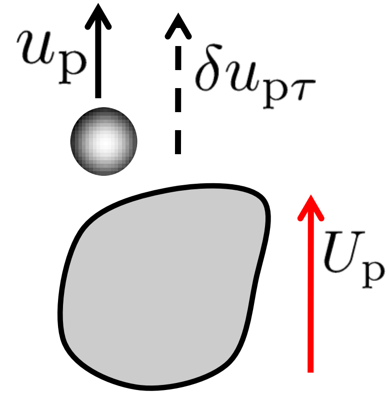
$u_{p\tau} = (1+\gamma)(U_p - u_p)$

Case 3



DO NOTHING

Case 4



if $u_p < U_p$

BUMP

$u_{p\tau} = (1+\gamma)(U_p - u_p)$

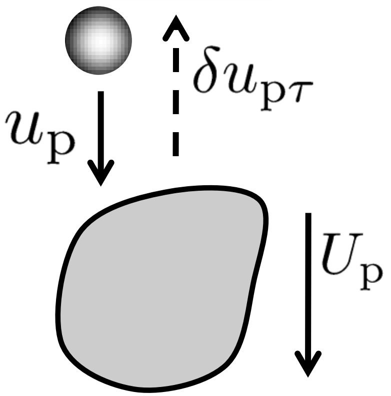
else

DO NOTHING

$$\mathbf{u}_p^{n+1} = \tilde{\mathbf{u}}_p + \mathbf{u}_{p\tau} \qquad \delta\mathbf{u}_{p\tau} = -\frac{\Delta t \nabla\tau}{\rho_s \varepsilon_s}$$

$$(\nabla\tau).\mathbf{e}_k \leq 0$$
$$u'_{p\tau_k} = \min\left(\mathbf{e}_k \cdot \delta\mathbf{u}_{p\tau}, (1+\gamma)(\mathbf{U}_p - \mathbf{u}_p)\cdot\mathbf{e}_k\right)$$
$$u_{p\tau_k} = \max\left(u'_{p\tau_k}, 0\right)$$

Case 1



if $|u_\mathrm{p}| > |U_\mathrm{p}|$

REBOUND

$u_{\mathrm{p}\tau} = (1+\gamma)(U_\mathrm{p} - u_\mathrm{p})$

else

DO NOTHING

---

if $|u_\mathrm{p}| > |U_\mathrm{p}|$

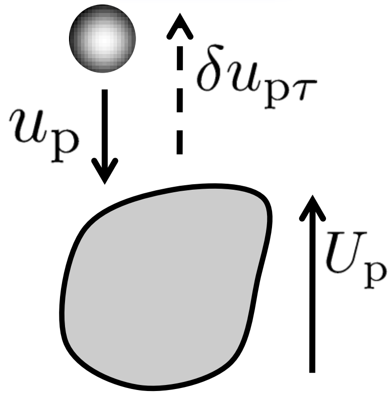
REBOUND

$u_\mathrm{p}^{n+1} = -e\, u_\mathrm{p}$

else

DO NOTHING

Case 2



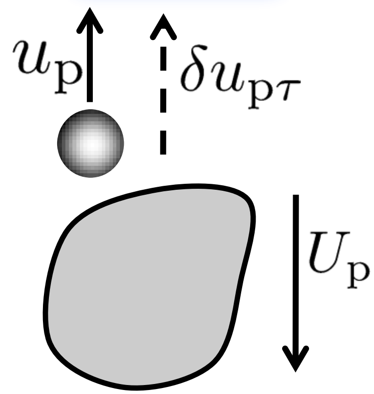
REBOUND

$u_{\mathrm{p}\tau} = (1+\gamma)(U_\mathrm{p} - u_\mathrm{p})$

REBOUND

$u_\mathrm{p}^{n+1} = -e\, u_\mathrm{p}$

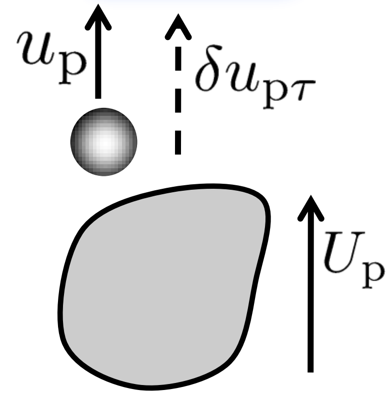
Case 3



DO NOTHING

DO NOTHING

Case 4



if $u_\mathrm{p} < U_\mathrm{p}$

BUMP

else

DO NOTHING

DO NOTHING

Implementation comparison

$$\boxed{m\frac{d\mathbf{u}_\text{p}}{dt} = m\mathbf{g} + \mathbf{f}_\text{p,drag} + m\mathbf{A}_\text{coll}}$$

Existing Literature

$$\mathbf{u}_\text{p}^{n+1} = \tilde{\mathbf{u}}_\text{p} + \mathbf{u}_{\text{p},\tau}$$

$$\tilde{\mathbf{u}}_\text{p} = \mathbf{u}_\text{p}^n + \left(\mathbf{g} + \frac{\mathbf{f}_\text{p,drag}}{m}\right)\Delta t$$

$$\mathbf{x}_\text{p}^{n+1} = \mathbf{x}_\text{p}^n + \Delta t\mathbf{u}_\text{p}^{n+1}$$

Wall B.C. on $\left(\mathbf{x}_\text{p}^{n+1}, \mathbf{u}_\text{p}^{n+1}\right)$?

Static friction ?

Snider, D. M., An incompressible 3-D MP-PIC model for dense particle flows, JCP (2001)

MFIX

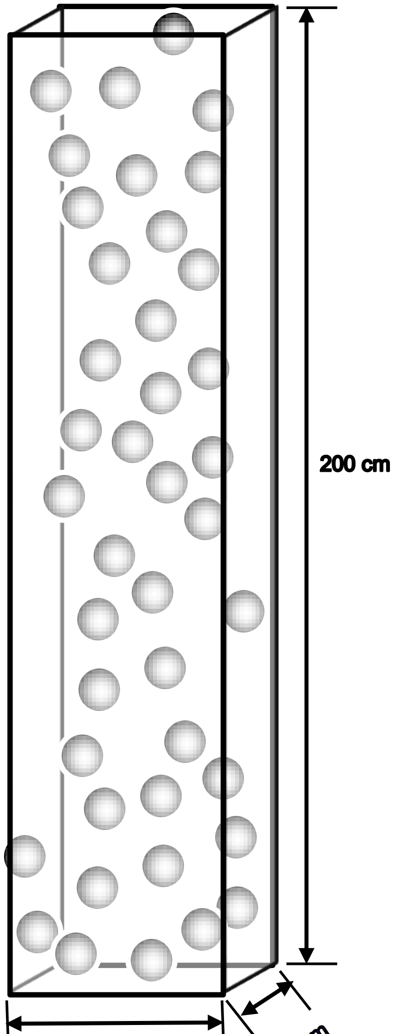
$$\mathbf{u}'^{n+1}_\text{p} = \mathbf{u}_\text{p}^n + \left(\mathbf{g} + \frac{\mathbf{f}_\text{p,drag}}{m}\right)\Delta t$$

$$\mathbf{x}'^{n+1}_\text{p} = \mathbf{x}_\text{p}^n + \Delta t\mathbf{u}'^{n+1}_\text{p}$$

$$\left(\mathbf{x}'^{n+1}_\text{p}, \mathbf{u}'^{n+1}_\text{p}\right) \xrightarrow[\text{Specular}]{\text{Wall B.C.}} \left(\mathbf{x}_\text{p}^{n+1}, \mathbf{u}^{*n+1}_\text{p}\right)$$

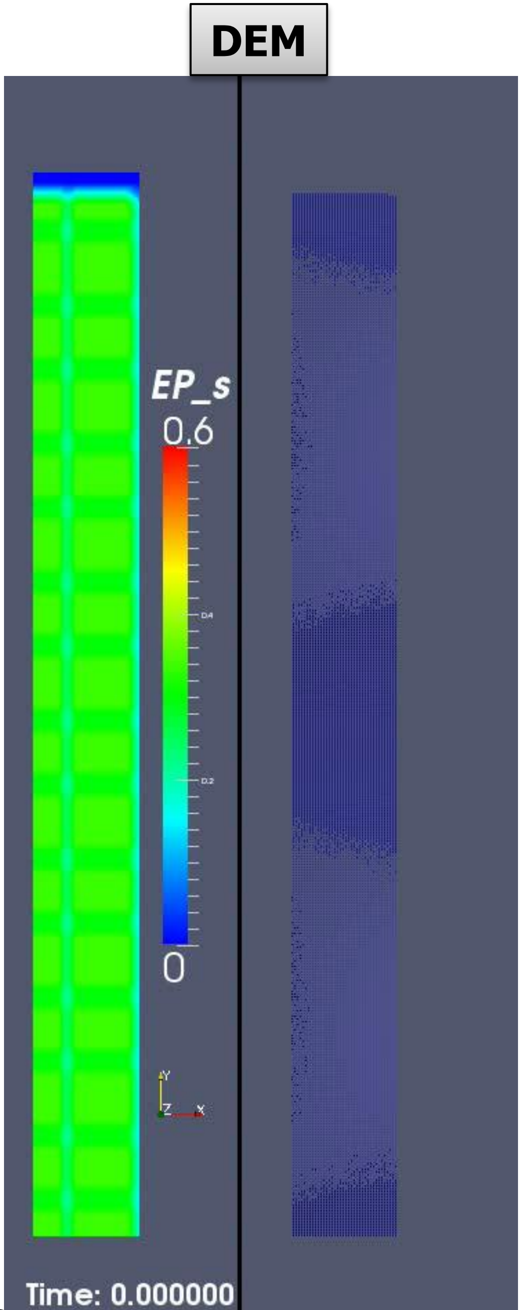
$$\mathbf{u}^{*n+1}_\text{p} \xrightarrow{A_\text{coll}} \mathbf{u}_\text{p}^{n+1}$$

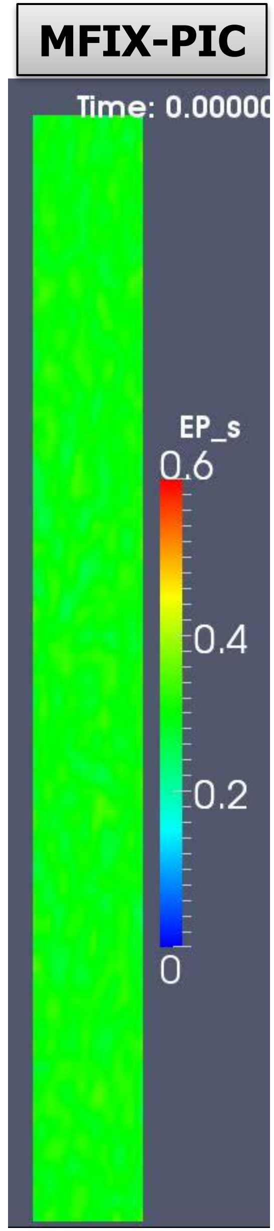
Sample Problem 1: Sedimentation



Properties
Solids: D_p = 0.4 cm, ρ_p = 2 g/cm^3 Initial solid volume fraction: 0.3 – 0.4 5 parcels per cell (2 particles per parcel)
Gas: Air at standard conditions
$e_{n,wall}$ = 0.8, $e_{t,wall}$ = 1.0
e_n = 0.6 (frictional A_{coll})
box dimension = (20x200x0.4) cm^3 ≡ (20x100x1) cells
DT = 1.E-02 – 1.E-04 sec
Drag model: Wen & Yu / Ergun

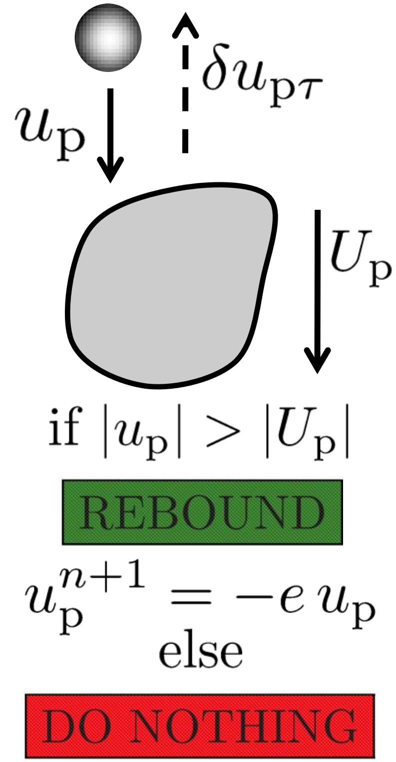
(Dt max=0.001)





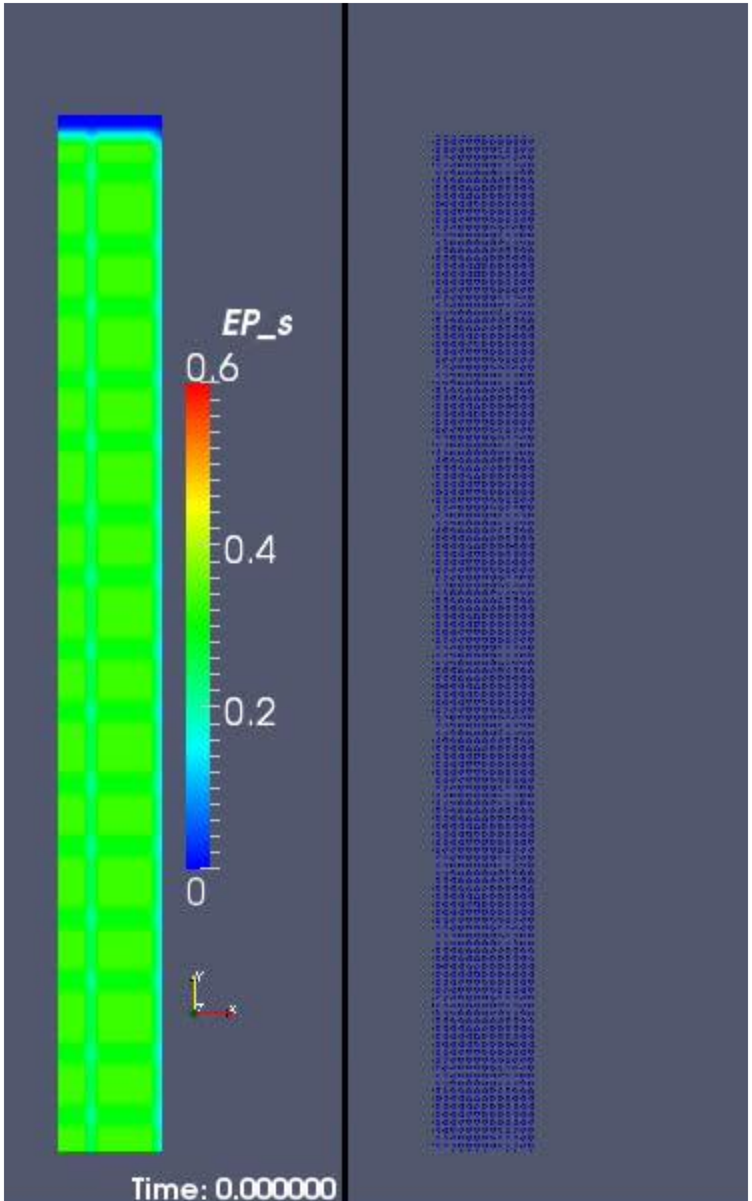
Stable simulation with rebound captured at the top

Case 1

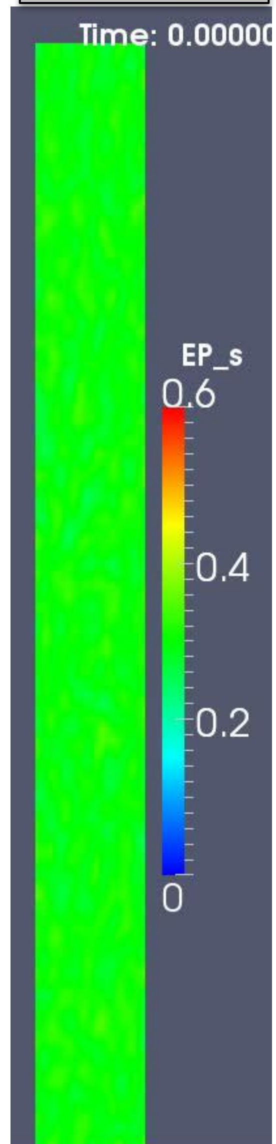


(Dt max=0.001)

DEM



MFIX-PIC



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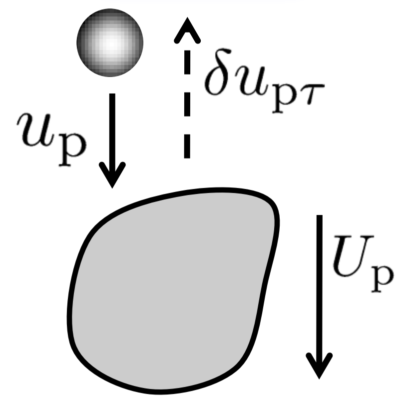
Case 1



if $|u_{\mathrm{p}}| > |U_{\mathrm{p}}|$

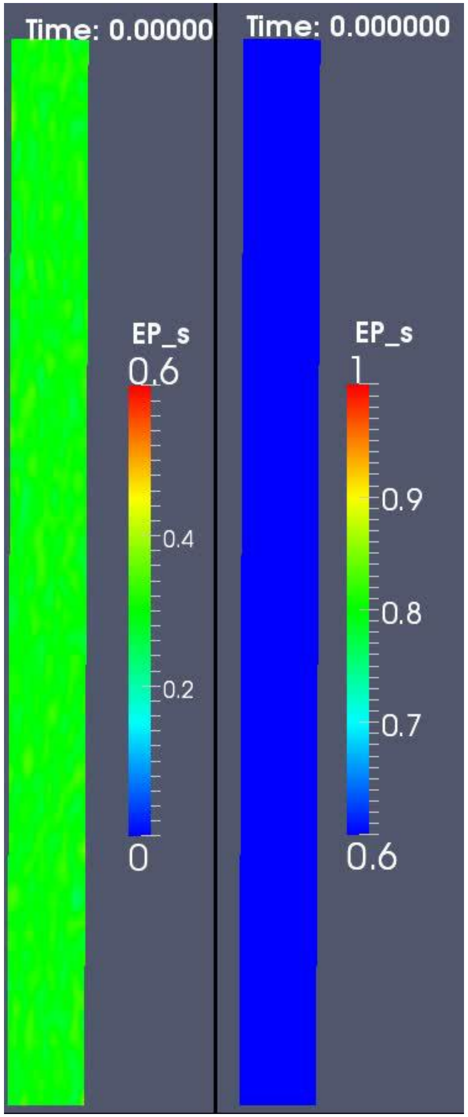
REBOUND

$$u_{\mathrm{p}}^{n+1} = -e\, u_{\mathrm{p}}$$

else

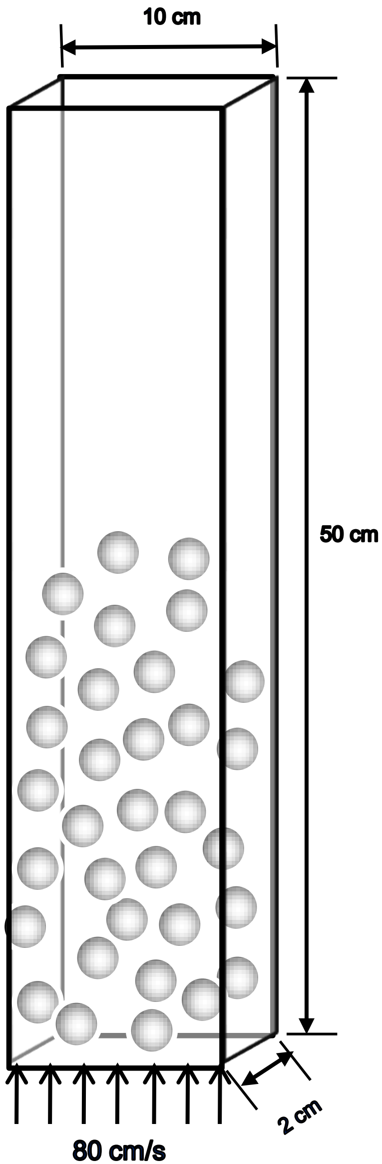
DO NOTHING

Effect of DT
DT max = 0.01



- ❑Over packing in the wall cells normal to gravity
  - ✓**not so much of a problem where there is a counter flow**

Sample Problem 2: bubbling bed

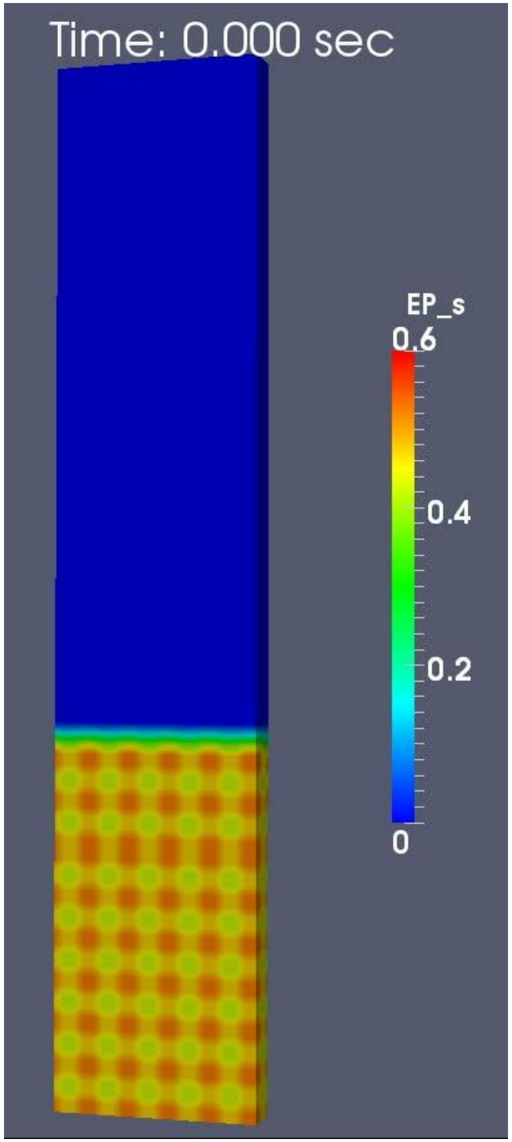


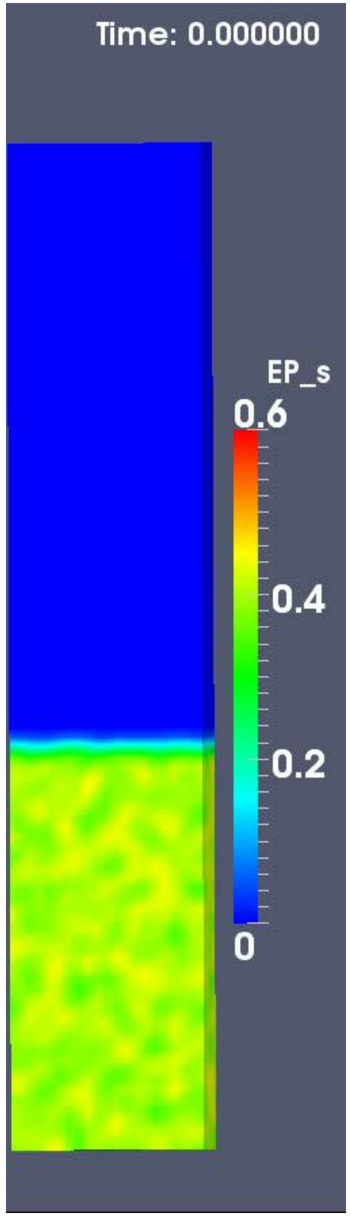
Properties
Solids: D_p = 0.1 cm, ρ_p = 2.5 g/cm^3 Initial solid volume fraction: 0.4 up to 20 cm 5 parcels per cell
Gas: Air at standard conditions Fluidization velocity = 80 cm/s
$e_{n,wall}$ = 0.8, $e_{t,wall}$ = 1.0
e_n = 0.8
box dimension = (10x50x2) cm^3 ≡ (20x100x4) cells
DT_{max} = 1.E-03
Drag model: Wen &Yu / Ergun

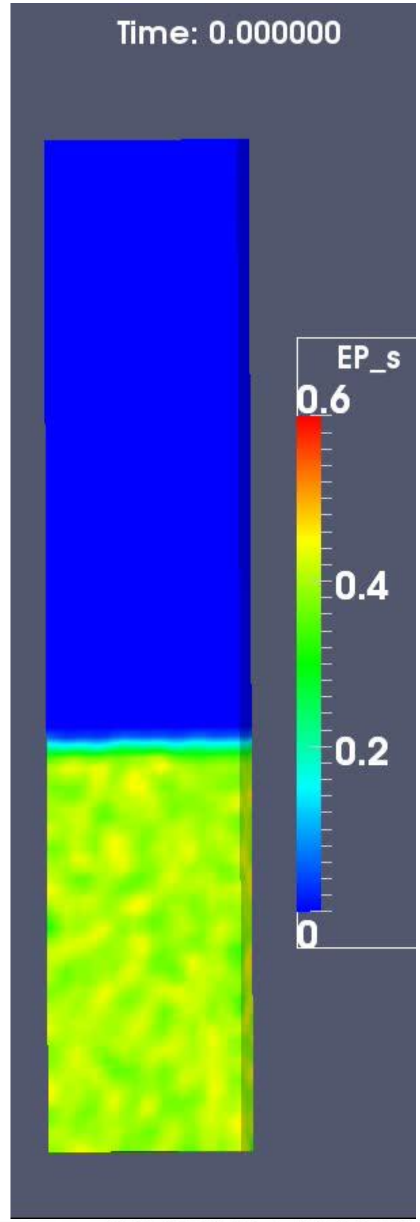
DEM

MFIX-PIC

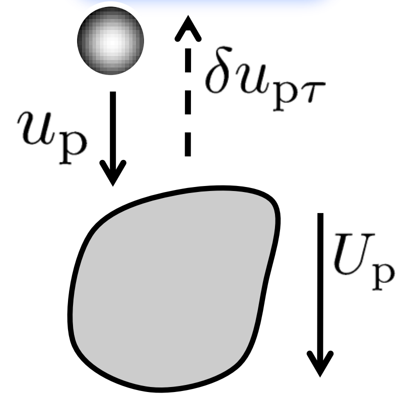
Small bubbles compared to DEM







Case 1B



if $|u_p| > |U_p|$

REBOUND

$$\cancel{u_p^{n+1} = -e\, u_p}$$

$$\boxed{u_p^{n+1} = e\, U_p}$$

else

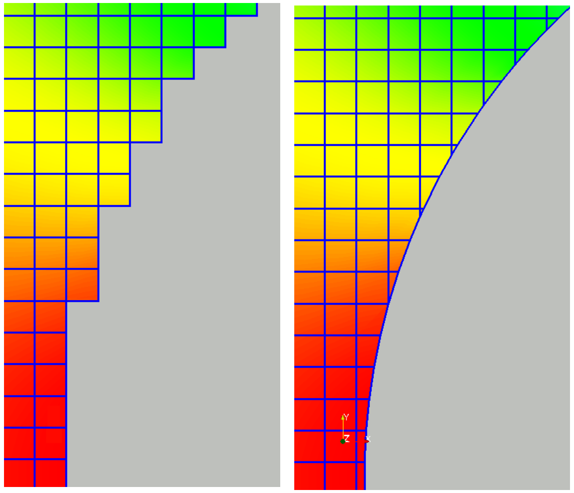
DO NOTHING

Conclusions/Observations

- **MPPIC model implemented in open-source MFIX code**
  - A new limiter based on physical arguments formulated for solid-stress model
- **The method is very sensitive to interpolation and/or sequence of particle trajectory equation integration**
- **Further work and independent V&V needed to establish *physics-based* rules for a *robust* solid-stress model**

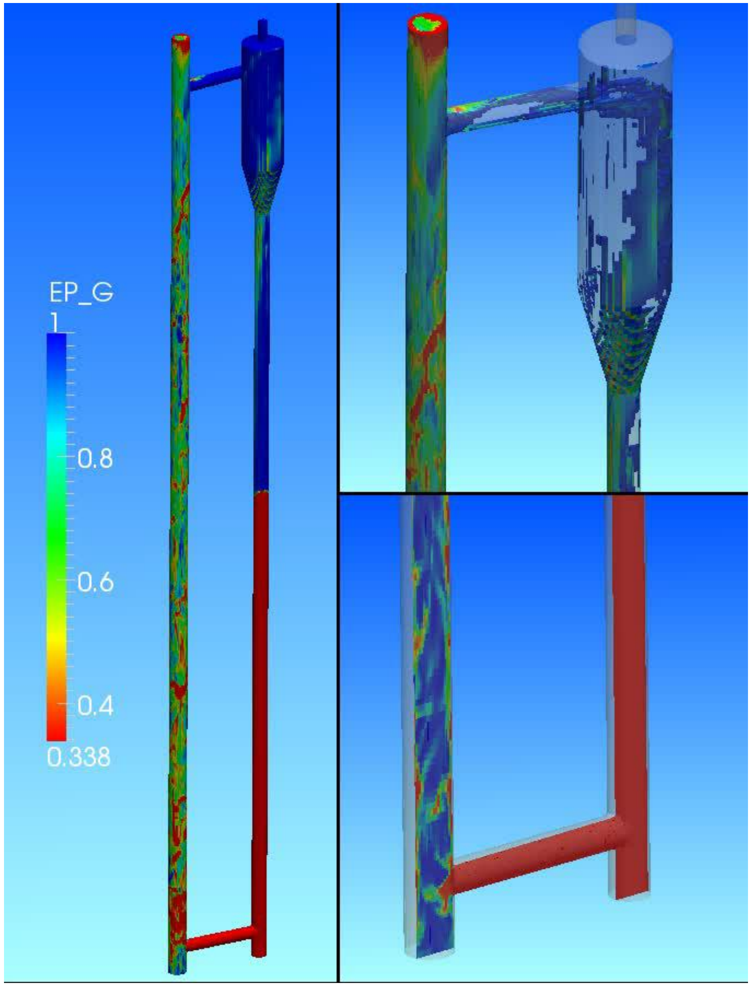
Extension to complex geometries

- MFIX is based on structured grid
- Complex geometries are represented in EE solver by cut-cell technique
- MPPIC implementation will use same cut cell technique to avoid staircase steps



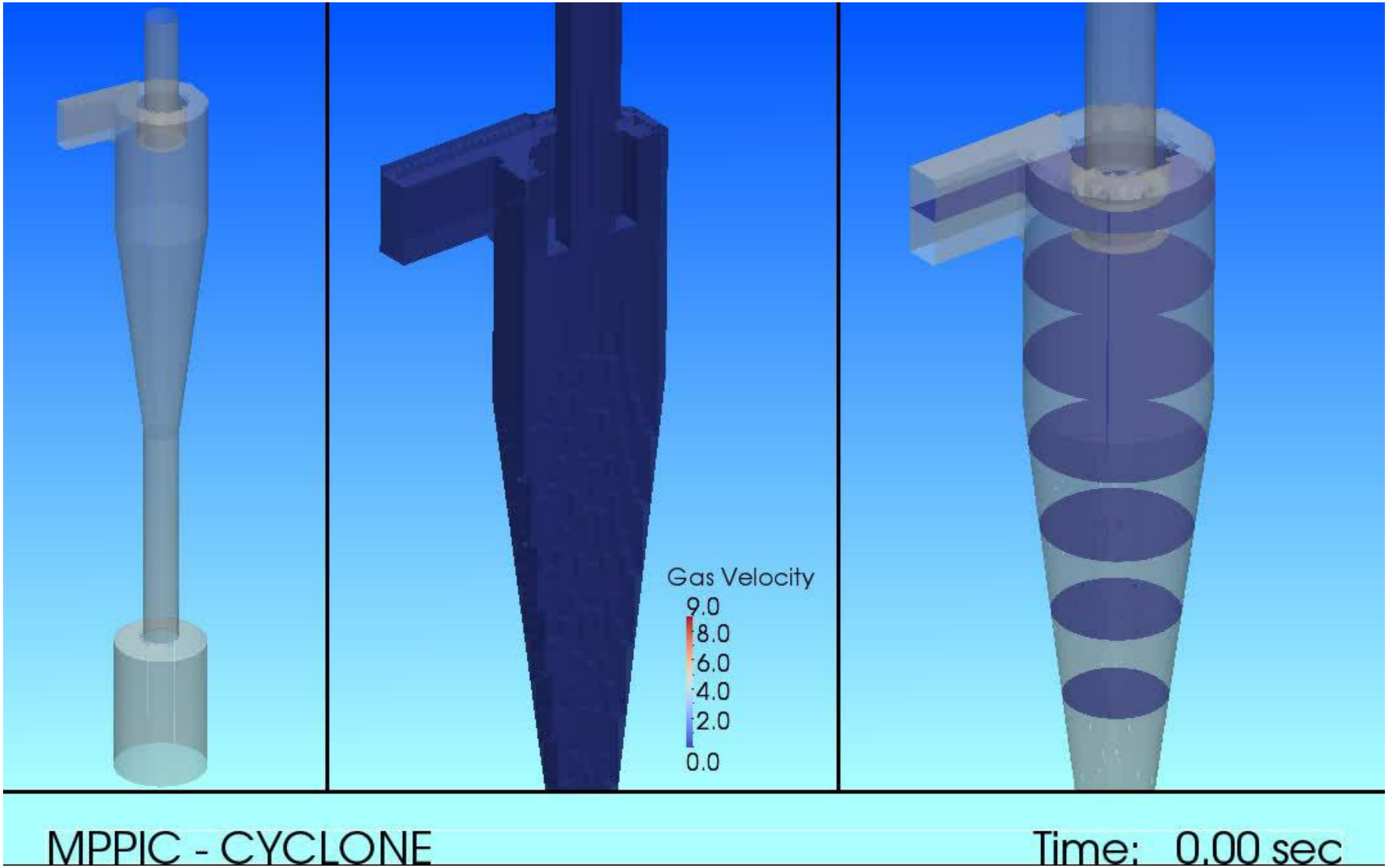
Staircase steps *Cut cells*

J. Dietiker, Cartesian Grid User Guide, https://mfix.netl.doe.gov



EE simulation of NETL CFB (Challenge problem)

Extension to complex geometries



Future work: extension to two-way coupling

Acknowledgments

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Thanks